

## Abstract

### Hydrogen Bonding and Stacking Interaction in Uracil Dimer. Comparison of (OVOS) CCSD(T), DFT-SAPT and DFT methods.

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CCSD(T) method is nowadays one of the most trusted methods for obtaining high accuracy results (at least for single reference ground states). However, its roughly  $N^6$  (and  $N^7$  for perturbative triples) scaling is prohibitive for applications in large systems.

It was shown by several authors that the scaling with respect to the number of virtual orbitals can be reduced by employing optimized orbitals (1), (2)... Though, this approach can lead to "an order of magnitude" acceleration of the CCSD(T) calculations, in combination with the available CCSD(T) codes, it quickly converges to the "hardware limit".

This was the reason for implementing a new, robust, parallel CCSD(T) algorithm without any extraordinary requirements on the computer memory. So far, the implementation is available without the point-group symmetry and for closed-shell molecules only (algorithm is based on (3)). The major difference with the standard codes, is that we use MO-transformed, Cholesky decomposed 2-el. integrals, which (together with  $T_2$  amplitudes and all pertinent auxiliary matrixes) are treated in "blocks".

We also present new results (and timings) of the (OVOS) CCSD(T), DFT-SAPT (4), DFT-D (5) and M06-2X (6) interaction energy calculations on the uracil dimer, as a model system for hydrogen bonding and stacking in DNA. Dimers are investigated not only in equilibrium distance, but also in stretched geometries to investigate the scaling of the interaction energy (components) with respect to the intermolecular distance.

1. P. Neogrady, M. Pitoňák and M. Urban, *Mol. Phys.* (2005) **103**, 2141.
2. A.G. Taube and R.J. Bartlett, *Collect. Czechoslov. Chem. Comm.* (2005) **70**, 837.
3. G.E. Scuseria, C.L. Janssen, H.F. Schaefer III, *J. Chem. Phys.* (1988) **89**, 7282.
4. A. Hesselmann, G. Jansen, M. Schutz, *J. Chem. Phys.* (2005) **122**, 1.
5. P. Jurecka, J. Cerny, P. Hobza, D.R. Salahub, *J. Comp. Chem* **28**, 555.
6. Y. Zhao, D.G. Truhlas, *Theor. Chem. Acc.* (2007) DOI 10.1007/s00214-0070310-x